

Exploring benzothiazole derivatives: Promising PLK1 Inhibitors for cancer therapy through Virtual screening, Molecular docking, and ADMET evaluation

Shivkant Patel*, Ashish Shah & Ashim Kumar Sen

Department of Pharmacy, Sumandeep Vidyapeeth Deemed to be University, Piparia, Vadodara-391 760, Gujarat, India

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Supplementary Data

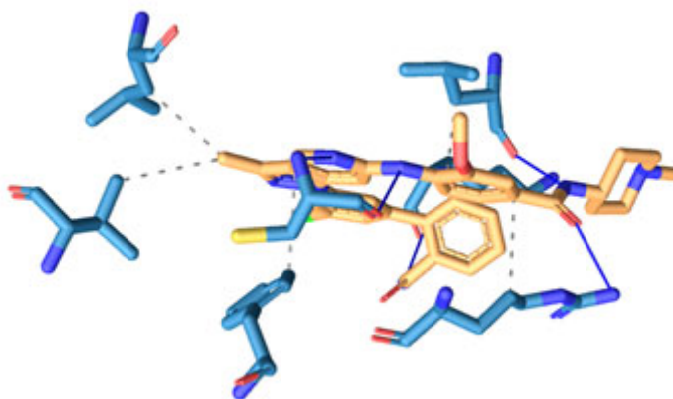
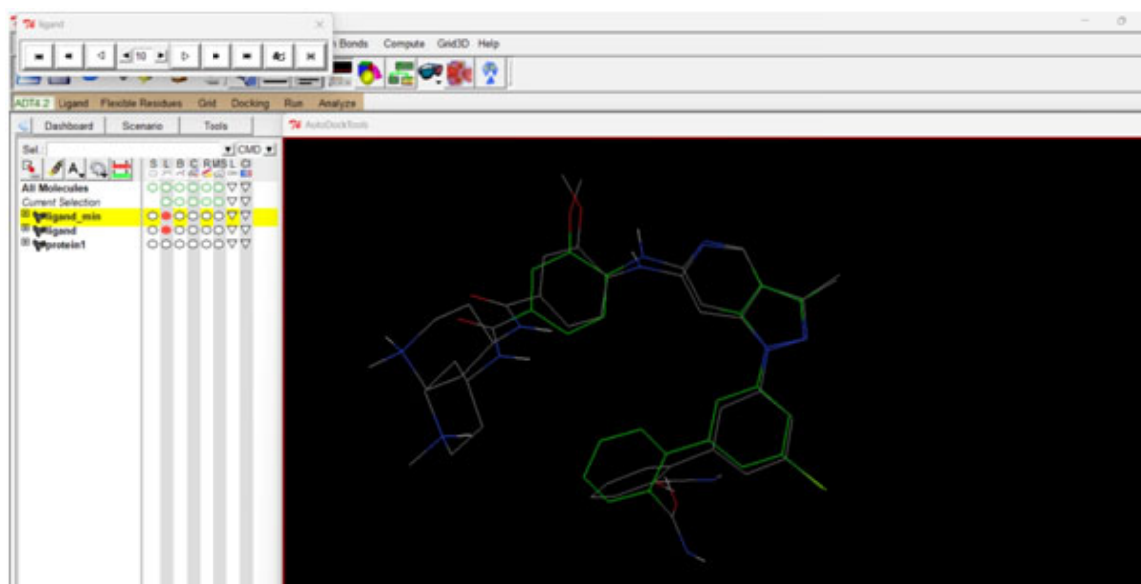


Fig. S1 — Amino Acid Interaction from PLIP server (3DBE)



Co-crystallized ligand— grey color, docked ligand--- green color

Fig. S2 — Docking of Ligand (Compound557) on Protein 3DBE

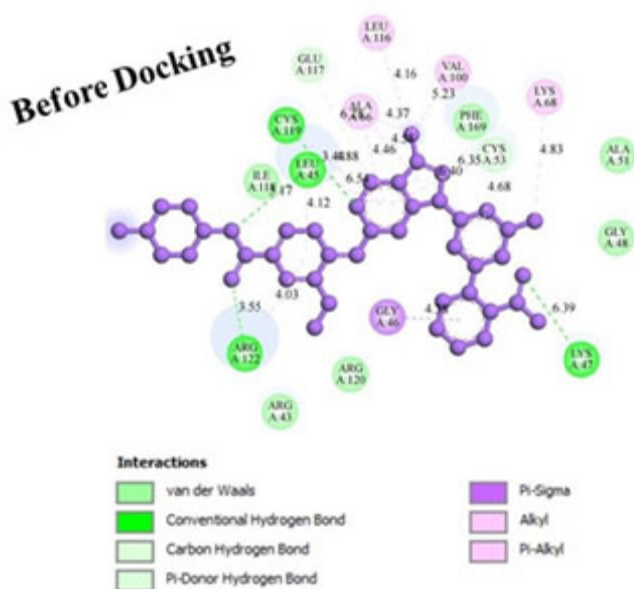


Fig. S3 — 2D interaction of ligand (Compound557) in binding pocket of 3DBE protein (before docking)

Table S1 — IUPAC Name and Smile strings of top 10 molecules

C. No.	PubChem ID/IUPAC	Smile
P1	PubChem CID 10779701 6-Fluoro-2-(3-methyl-4-nitrophenyl)-1,3-benzothiazole	<chem>O=[N+](C1=CC=C(C2=NC3=CC=C(F)C=C3S2)C=C1C)[O-]</chem>
P2	PubChem CID 10946124 2-(3-Methyl-4-nitrophenyl)-7-fluorobenzothiazole	<chem>FC1=C(SC(C2=CC=C([N+](O-))=O)C(C)=C2)=N3)C3=CC=C1</chem>
P3	PubChem CID 153949097 2-(4b-Methyl-5,6,7,8-tetrahydrocarbazol-3-yl)-1,3-benzothiazole	<chem>CC12C3=C(C=CC(C4=NC5=CC=CC=C5S4)=C3)N=C1CCCC2</chem>
P4	PubChem CID 15880521 2-(3-Methyl-4-nitrophenyl)-5-fluorobenzothiazole	<chem>FC1=CC=C(SC(C2=CC=C([N+](O-))=O)C(C)=C2)=N3)C3=C1</chem>
P5	PubChem CID 137735789 6-(1,3-Benzothiazol-2-yl)-1,2,2,4-tetramethyl-1,2-dihydroquinoline	<chem>CC1=CC(C)(C)N(C)C2=C1C=C(C3=NC4=CC=CC=C4S3)C=C2</chem>
P6	PubChem CID 15880522 2-(3-Methyl-4-nitrophenyl)-5,6-difluorobenzothiazole	<chem>FC1=C(F)C=C2N=C(C3=CC=C([N+](O-))=O)C(C)=C3)SC2=C1</chem>
P7	PubChem CID 10566560 2-(3-Methyl-4-nitrophenyl)-4,6-difluorobenzothiazole	<chem>FC1=CC(F)=C2N=C(C3=CC=C([N+](O-))=O)C(C)=C3)SC2=C1</chem>
P8	PubChem CID10589414 4-Fluoro-2-(3-methyl-4-nitrophenyl)-1,3-benzothiazole	<chem>O=[N+](C1=CC=C(C2=NC3=C(F)C=CC=C3S2)C=C1C)[O-]</chem>
P9	PubChem CID 159531422 1-[4-(1,3-benzothiazol-2-yl)-2-methylphenyl]-4,6-dimethyl-2H-pyrimidin-2-amine	<chem>NC1N=C(C)C=C(C)N1C2=CC=C(C3=NC4=CC=CC=C4S3)C=C2C</chem>
P10	PubChem CID10542666 4,5-Difluoro-2-(3-methyl-4-nitrophenyl)-1,3-benzothiazole	<chem>O=[N+](C1=CC=C(C2=NC3=C(F)C(F)=CC=C3S2)C=C1C)[O-]</chem>
5f-203	4-(5-fluorobenzo[d]thiazol-2-yl)-2-methylaniline	<chem>FC1=CC=C(SC(C2=CC=C(N)C(C)=C2)=N3)C3=C1</chem>

Table S2 — Interacting amino acid residues involved for the hit-compounds bound to PLK protein

C. No.	Hydrogen bond	Carbon Hydrogen bond	Hydrophobic Interaction		Electrostatic	
			π -sigma	π -alkyl	π -Sulfur	Fluorine
5f-203	Arg120	-	-	Ala66, Arg122, Ile118	-	-
P1	Arg43, Cys119	-	Leu45	Val100, Phe169, Leu116	Cys53, Cys111	-
P2	Arg43, Cys119	-	Leu45	Ile118, Arg122	Phe169, Cys119	-
P3	-	-	Leu45	Phe169, Val100, Leu 116	Lys53	-
P4	Arg43, Cys119	-	Leu45	Ala66, Arg122	Cys53	Glu117
P5	Cys53	-	Leu45	Arg122, Arg120, Ile118, Ala66, Leu116, Val100	Cys119	-
P6	Arg43, Cys119	-	Leu45	Cys53, Ala66, Arg120, Arg122, Ile118	Cys119	Glu117
P7	Arg43, Cys119	Lys68	Leu45	Ala66, Arg120	Cys53	Glu117, Ile118
P8	Arg43, Cys119	-	Leu45	Cys53, Ala66, Arg120	-	Glu117, Ile118
P9	Glu126	Gly166	Leu45, Arg120	Leu125, Phe169	-	-
P10	Arg43, Cys119	-	Leu45	Cys53, Ala66, Arg120	Cys119	Glu117, Ile118

Table S3 — Docking score and IUPAC name of newly designed compounds

C. No.	IUPAC Name	Score in (Kcal/mol)
N1	6-fluoro-2-(1,2,2,4-tetramethyl-1,2-dihydroquinolin-6-yl) benzo[d]thiazole	-8.48
N2	1-(4-(6-fluorobenzo[d]thiazol-2-yl)-2-methylphenyl)-4,6-dimethyl-1,2-dihydropyrimidin-2-amine	-7.95
N3	7-fluoro-2-(1,2,2,4-tetramethyl-1,2-dihydroquinolin-6-yl) benzo[d]thiazole	-8.38
N4	1-(4-(7-fluorobenzo[d]thiazol-2-yl)-2-methylphenyl)-4,6-dimethyl-1,2-dihydropyrimidin-2-amine	-7.94
N5	6,7-difluoro-2-(1,2,2,4-tetramethyl-1,2-dihydroquinolin-6-yl) benzo[d]thiazole	-8.41
N6	1-(4-(6,7-difluorobenzo[d]thiazol-2-yl)-2-methylphenyl)-4,6-dimethyl-1,2-dihydropyrimidin-2-amine	-7.99